JOURNAL OF MOLECULAR RECOGNITION (*J. Mol. Recogn.*)

CONTENTS

Volume 9 Numbers 1–6

Number 1 January/February 1996

Automated Docking of Flexible Ligands: Applications of AutoDock
D. S. Goodsell, G. M. Morris and A. J. Olson 1

The Effect of Water Activity on the Association Constant and the Enthalpy of Reaction Between Lysozyme and the Specific Antibodies D1.3 and D44.1
F. A. Goldbaum, F. P. Schwarz, E. Eisenstein, A. Cauerhff, R. A. Mariuzza and R. J. Poljak 6

***Lac* Repressor–Operator Interaction: *N*-Terminal Peptide Backbone ^{1}H and ^{15}N Chemical Shifts upon Complex Formation with DNA**
P. G. Artz, K. G. Valentine, S. J. Opella and P. Lu 13

Roles of Lysine-69 in Dimerization and Activity of *Trimeresurus flavoviridis* Venom Aspartate-49-phospholipase A_2
S. Nakamura, M. Nakai, K.-I. Nakashima, T. Ogawa, Y. Shimohigashi, M. Ohno, H. Kihara, T. Yamane and T. Ashida 23

Binding of Fibrogen to Platelet Integrin αIIBβ3 in Solution as Monitored by Tracer Sedimentation Equilibrium
G. Rivas, K. Tangemann, A. P. Minton and J. Engel 31

Comparative Interaction Kinetics of Two Recombinant Fabs and of the Corresponding Antibodies Directed to the Coat Protein of Tobacco Mosaic Virus
J. Chatellier, N. Rauffer-Bruyère, M. H. V. Van Regenmortel, D. Altschuh and E. Weiss 39

Number 2 March/April 1996

MOLECULAR RECOGNITION IN DRUG DISCOVERY
Based on the 36th Annual Buffalo Medicinal Chemistry Symposium
Guest Editors: A. W. Czarnik and A. V. Eliseev

Guest Editorial
A. W. Czarnik 53

Molecular Recognition by Natural Macrocycles. I. d-Tubocurarine as a Host Molecule for Organic Anions
C. G. Alcántar, A. V. Eliseev and A. K. Yatsimirsky 54

Molecular Interaction Analysis in Ligand Design Using Mass Transport, Kinetic and Thermodynamic Methods
M. L. Doyle, D. G. Myszka and I. M. Chaiken 65

Specific Targeting of Protein–DNA Complexes by DNA Reactive Drugs (+)-CC-1065 and Pluramycins
D. Henderson and L. H. Hurley 75

The '*n*' Effect in Molecular Recognition
M. S. Westwell, M. S. Searle and D. H. Williams 88

A Molecular Dynamics Study of the Three-Dimensional Model of Human Synovial Fluid Phospholipase A_2—Transition State Mimic Complexes
V. Hariprasad and V. M. Kulkarni 95

A Technique to Study Molecular Recognition in Drug Design: Preliminary Application of Free Energy Derivatives to Inhibition of a Malarial Cysteine Protease
P. Cieplak and P. A. Kollman 103

Seeing Double: Crystal Structures of the Type I TNF Receptor 113
J. H. Naismith, B. J. Brandhuber, T. Q. Devine and S. R. Sprang

Comparative *in vivo* Sensitizing Efficacy of Porphyrin and Chlorin Dimers Joined with Ester, Ether, Carbon–Carbon or Amide Bonds
R. K. Pandey, G. Zheng, D. A. Lee, T. J. Dougherty and K. M. Smith 118

Experimental Results from Host–Guest Complexes for the Design of Effectors in Biological Systems and of Enzyme Analogous Catalysts
H.-J. Schneider, F. Eblinger, J. Sartorius and J. Rammo 123

Molecular Similarity Analysis on Biologically Active Macrocyclic Bis(bibenzyls)
G. M. Keserű and M. Nógrádi 133

Inhibitors of HIV Protease: Unique Non-peptide Active Site Templates
B. D. Tait, J. Domagala, E. L. Ellsworth, D. Ferguson, C. Gajda, D. Hupe, E. A. Lunney and P. J. Tummino 139

Hydrophobic vs Coulombic Interactions in the Binding of Steroidal Polyamines to DNA
J. G. Muller, M. M. P. Ng and C. J. Burrows 143

Molecular Recognition with C-Clamp Porphyrins: Synthesis, Structural, and Complexation Studies
Y. Liang, C. K. Chang and S.-M. Peng 149

Model Systems for Flavoenzyme Activity. The Effects of Specific Hydrogen Bonds on the ^{13}C and ^{1}H NMR of Flavins
A. Niemz and V. M. Rotello 158

All D-Amino Acid Hexapeptide Inhibitors of Melittin's Cytolytic Activity Derived from Synthetic Combinatorial Libraries
S. E. Blondelle, R. A. Houghten and E. Pérez-Payá 163

Novel Nonclassical Inhibitors of Glycinamide Ribonucleotide Formyltransferase: 10-Formyl and 10-Hydroxymethyl Derivatives of 5,8,10-Trideazapteroic Acid
L. Liu, M. G. Nair and R. L. Kisliuk 169

Molecular Docking Towards Drug Discovery
D. A. Gschwend, A. C. Good and I. D. Kuntz 175

Design and Analysis of RNA Structure-Specific Agents as Potential Antivirals
W. D. Wilson, L. Ratmeyer, M. Zhao, D. Ding, A. W. McConnaughie, A. Kumar and D. W. Boykin 187

Inhibition of Phosphatidyl Inositol-Specific Phospholipase C: Studies on Synthetic Substrates, Inhibitors and a Synthetic Enzyme
D. Vizitiu, A. G. Kriste, A. S. Campbell and G. R. J. Thatcher 197

Number 3 May/June 1996

REVIEW PAPER
Review of Conformation-Specific Affinity Purification Methods for Plasma Vitamin K-dependent Proteins
S. B. Yan 211

Enhanced Uranyl Photocleavage Across the Minor Groove of All $(A/T)_4$ Sequences Indicates a Similar Narrow Minor Groove Conformation
S. H. Sönnichsen and P. E. Nielsen 219

Sequence/Structure Selective Thermal and Photochemical Cleavage of yeast-$tRNA^{Phe}$ By UO_2^{2+}
P. E. Nielsen and N. E. Møllegaard 228

Characteristics of β-adrenergic Receptors in Longitudinal Muscle Membranes of Rat Uterus: Changes in Kinetic Properties of the Receptor During Gestation
Y. Kaneko, T. Tsukamoto, T. Kawarabayashi, M. Ikeda and H. Sugimori 233

Prediction of IgE(Lb4)–Ligand Complex Structures by Automated Docking
R. H. Winger, K. R. Liedl, C. A. Sotriffer, A. M. Gamper, B. M. Rode, R. T. Kroemer and J. M. Varga 239

Fibrinogen Adsorption to Receptor-Like Biomaterials Made by Pre-adsorbing Peptides to Polystyrene Substrates
J. M. Grunkemeier and T. A. Horbett 247

Announcement 258

Number 4 July/August 1996

REVIEW PAPER

Dye-Affinity Techniques for Bioprocessing: Recent Developments
N. Garg, I. Yu. Galaev and B. Mattiasson 259

Three-Dimensional Model of a Selective Theophylline-Binding RNA Molecule
C.-S. Tung, T. I. Oprea, G. Hummer and A. E. García 275

β-Lactam Drug Allergens: Fine Structural Recognition Patterns of Cephalosporin-Reactive IgE Antibodies
N. H. Pham and B. A. Baldo 287

Chelation-Enhanced Fluorescence Chemosensing of Pb(II), an Inherently Quenching Metal Ion
M.-Y. Chae, J. Yoon and A. W. Czarnik 297

Numbers 5/6 September/December 1996

11th INTERNATIONAL SYMPOSIUM ON AFFINITY CHROMATOGRAPHY AND BIOLOGICAL RECOGNITION
Guest Editor: W. H. Scouten

CRITICAL REVIEWS

Screening for Protein Purification: is there an Optimum Adsorbant for every Protein
R. K. Scopes 305

Biorecognition of Antibodies *in vivo*: Potential in Drug Targeting
A. R. Fritzberg 309

Principles and Applications of Flow Injection Analysis in Biosensors
E. H. Hansen 316

New Formats of Polymeric Stationary Phases for HPLC Separations: Molded Macroporous Disks and Rods
F. Svec and J. M. J. Fréchet 326

Affinity Liposomes *in vivo*: Factors Influencing Target Accumulation
V. P. Torchilin 335

Interleukin 5 Interactions with Soluble and Cell Surface Forms of its Receptor
J. Li, R. Cook and I. Chaiken 347

Affinity Precipitation of Proteins
M. N. Gupta, R. Kaul, D. Guoqiang, U. Dissing and B. Mattiasson 356

Detection of Pathological Changes of Proteins by Peptide Mapping after Protein Digestion by Use of Oriented Immobilized Proteinases
J. Turková, Z. Kučerová and M. J. Beneš 360

RESEARCH ARTICLES

Two Lectin-like Receptors for α_1-acid Glycoprotein in Mouse Testis
U. O. Andersen, S. Kirkeby and T. C. Bøg-Hansen 364

Membrane Microstructural Templates for Enzyme Domain Formation
K. M. Maloney, M. Grandbois, C. Salesse, D. W. Grainger and A. Reichert 368

Salicylaldehyde–metal–amino Acid Ternary Complex: A New Tool for Immobilized Metal Affinity Chromatography
D. Leibler, A. Rabinkov and M. Wilchek 375

Reversible and Irreversible Immobilization of Enzymes on Graphite Fibrils™
L. Dong, A. B. Fischer, M. Lu, M. T. Martin, D. Moy and D. Simpson 383

Immobilised Metal-ion Affinity Chromatography: Imidazole Proton Pump and Chromatographic Sequelae. I. Proton Pump
E. Sulkowski 389

Polyvinyl Alcohol-coated Perfluorocarbon Supports for Metal Chelating Affinity Separation of a Monoclonal Antibody
P. E. Morgan, O. R. T. Thomas, P. Dunnill, A. J. Sheppard and N. K. H. Slater 394

Affinity of Human Anti-factor VIII Antibodies for Functional Polystyrene Supports
L. Dahri, J. F. Stoltz, C. Boisson-Vidal, D. Muller and J. Jozefonvicz 401

Affinity Purification of Biologically Active and Inactive Forms of Recombinant Human Proteins C Produced in Porcine Mammary Gland
K. E. Van Cott, B. Williams, W. H. Velander, F. Gwazdauskas, T. Lee, H. Lubon and W. N. Drohan 407

Alginate as a Displacer for Protein Displacement Chromatography
G. Chen and W. H. Scouten 415

Peptides as Affinity Surfaces for Protein Purification
A. Pingali, B. McGuinness, H. Keshishian, J. Fei-Wu, L. Varady and F. Regnier 426

Coprecipitation of Proteins with Matrix Ligands: Scaleable Protein Isolation
D. Matulis, R. Lovrien and T. I. Richardson 433

Human Low Density Lipoprotein and Human Serum Albumin Adsorption onto Model Surfaces Studied by Total Internal Reflection Fluorescence and Scanning Force Microscopy
C.-H. Ho, D. W. Britt and V. Hlady 444

Determination of Binding Constants of Diabodies Directed against Prostate-specific Antigen using Electrochemiluminescence-based Immunoassays
R. Abraham, S. Buxbaum, J. Link, R. Smith, C. Venti and M. Darsley 456

Studies on Oriented and Reversible Immobilization of Glycoprotein using Novel Boronate Affinity Gel
X.-C. Liu and W. H. Scouten 462

Binding of *Escherichia coli* LexA Repressor to the *RecA* Operator
S. L. Shaner and E. S. Gaissarian 468

Development of an Immunomagnetic Assay System for Rapid Detection of Bacteria and Leukocytes in Body Fluids
J. G. Bruno, H. Yu, J. P. Kilian and A. A. Moore 474

Preliminary Investigations of an Amperometric Oligosaccharide Dehydrogenase-based Electrode for the Detection of Glucose and Some Other Low Molecular Weight Saccharides
T. Ruzgas, E. Csöregi, I. Katakis, G. Kenausis and L. Gorton 480

Immobilization of Streptavidin for Immunosensors on Nanostructured Surfaces
S. Kossek, C. Padeste and L. Tiefenauer 485

Structural Characterization and 5′-mononucleotide Binding of Polyalanine β-sheet Complexes
E. Pérez-Payá, B. Forood, R. A. Houghten and S. E. Blondelle 488

Immobilized Metal-ion Affinity Chromatography: Imidazole Proton Pump and Chromatographic Sequelae. II. Chromatographic Sequelae
E. Sulkowski 494

A Non-radioactive Assay System for Screening for Inhibitors of RNA-dependent Reverse Transcriptase Activity; an Analysis using Aurintricarboxylic Acid and Plant Flavonoids
G. Spedding 499

Monitoring Fibrinogen Adsorption Kinetics by Interfacial TIRF Rheometry
A. Sanders and H. P. Jennissen 503

Polymer-shielded Dye-affinity Chromatography
B. Mattiasson, I. Yu. Galaev and N. Garg 509

Cyclodextrin-aided Capillary Electrophoretic Separation and Laser-induced Fluorescence Detection of Polynuclear Aromatic Hydrocarbons (PAHs)
R. S. Brown, O. H. J. Szolar and J. H. T. Luong 515

Single Nucleotide Modulation of Uridine to Pseudouridine Rearrangement in Transfer RNA Catalyzed by Pseudouridine Synthase I
J. W. Chihade and D. A. Horne 524

Effect of Antibody Orientation on Immunosorbent Performance
A. Subramanian and W. H. Velander 528

***In vivo* Targeting of Colloidal Carriers by Novel Graft Copolymers**
R. Arshady 536

Dihydrofolate Reductase Synthesis in the Presence of Immobilized Methotrexate. An Approach to a Continuous Cell-free Protein Synthesis System
E. Marszal and W. H. Scouten 543

Synthesis and Characterization of Sol–Gel Phase-reversible Hydrogels Sensitive to Glucose
S. J. Lee and K. Park 549

Immobilization of Conalbumin onto Polystyrene/divinylbenzene Co-polymers: Towards Finding the Best Support for MAMC
E. Gonzalez-Vergara and J. B. Vincent 558

Protein A Mimetic Peptide Ligand for Affinity Purification of Antibodies
G. Fassina, A. Verdoliva, M. R. Odierna, M. Ruvo and G. Cassini 564

Sequence of Bifurcations in an 'Antigen–Antibody' Reaction
G. V. Grushevskaja and A. I. Khmelnitsky 570

Application of Perfluorocarbons in Novel Continuous Counter-current Protein Chromatography
R. O. Owen, G. E. McCreath and H. A. Chase 575

Multiple Affinity Domains for the Detection, Purification and Immobilization of Recombinant Proteins
J. Nilsson, M. Larsson, S. Ståhl, P.-Å. Nygren and M. Uhlén 585

Intermolecular Chiral Recognition Probed by Enantiodifferential Excited-state Quenching Kinetics
T. G. Stockman, C. A. Klevickis, C. M. Grisham and F. S. Richardson 595

Affinity Adsorption of *Saccharomyces cerevisiae* on Concanavalin A Perfluorocarbon Emulsions
G. E. McCreath and H. A. Chase 607

The Engineering of Biomaterials Exhibiting Recognition and Specificity
B. D. Ratner 617

'Wiring' of Lactate Oxidase within a Low-redox Potential Electron-conducting Hydrogel
G. Kenausis, C. Taylor, R. Rajagopalan and A. Heller 626

Epitope Contiguous Chains and Antibody Recognition in HIV-1 Synthetic Peptide Antigens
M. Aleanzi, N. Perotti, A. Montaner, J. Lottersberger, G. Tonarelli and A. Marcipar 631

Discriminatory Recognition of Membrane Phospholipids by Lysine-49-phospholipases A_2 from *Trimeresurus flavoviridis* Venom
Y. Shimohigashi, A. Tani, Y. Yamaguchi, T. Ogawa and M. Ohno 639

Novel Method for Coupling of Poly(ethyleneglycol) to Carboxylic Acid Moieties of Proteins
E. Kynclova, E. Elsner, A. Köpf, G. Hawa, T. Schalkhammer and F. Pittner 644

Some Recent Developments in the Preparation of Novel Recognition Systems: a Recognition Site for the Selective Catalysis of an Aldol Condensation using Molecular Imprinting and Specific Affinity Motifs for α-chymotrypsin using a Phage Display Peptide Library
I. A. Nicholls, J. Matsui, M. Krook and K. Mosbach 652

Biosensors in Flow-injection Systems for Biomedical Analysis, Process and Environmental Monitoring
C. Tran-Minh 658

New Technologies for Amperometric Biosensors
M. G. Boutelle, H. Allen, O. Hill, M. Berners, R. John, P. D. Dobson and P. Leigh 664

Five-membered Mercaptoheterocyclic Ligands for Thiophilic Adsorption Chromatography
A. Schwarz 672

Study of the Nature of Recognition in Molecularly Imprinted Polymers
H. S. Andersson, A.-C. Koch-Schmidt, S. Ohlson and K. Mosbach 675

Oriented Immobilization of Restriction Endonuclease EcoRI
M. Bircakova, M. Truksa and W. H. Scouten 683

Chiral Recognition in Adrenergic Receptor Binding Mimics Prepared by Molecular Imprinting
O. Ramström, C. Yu and K. Mosbach 691

Size-exclusion Phases and Repulsive Protein–polymer Interaction/recognition
D. E. Brooks and W. Müller 697

Diazotizable Supports of Potential Interest as Affinity Chromatography Matrices
M. J. Beneš, J. Lenfeld and O. Přádová 701

Effect of Immobilization on the Penicillin Binding and Reactivity Properties of DD-peptidase from *Streptomyces* R61
G. Y. Eng and R. J. Maxwell 706

Copper Binding Studies of Lipases from Different Sources using Image Binding: Mechanism of Free Copper and Chelated Copper
C. Colin and M. A. Vijayalakshmi 715

Purification and Identification of ABA-binding Proteins and Antibody Preparation
Y. Wan and K. H. Hasenstein 722

Well Defined Dye Adsorbents for Protein Purification
J. Scoble and R. Scopes 728

Interactions and Applications of Soluble Heterobifunctional Affinity Chelating Polymers in Immobilized Metal Affinity Chromatography
G. Ehteshami, J. Porath and R. Guzmán 733

Analysis of Antibody Selection by Phage Display Utilizing Anti-phenobarbital Antibodies
J. Malone and M. A. Sullivan 738

EXTENDED ABSTRACT

Analysis of Activated Components of the Complement System Using Optical Biosensor Techniques
M. Hibbs, A. Laver, A. Freeman and R. Smith 746

SHORT COMMUNICATIONS

Purification of an Expressed Insect Transferrin From Cell Culture Media Using High Capacity Ni^{2+}-DPA Gel
J. J. Winzerling, D. Q.-D. Pham, S. Kunz, J. H. Law and J. Porath 747

End Point Attached Heparin Affinity Matrix
L. K. LaFrance and J. Dapron 748

IN MEMORIAM

Christian B. Anfinsen (1916–1995)
Meir Wilchek 752

Author Index 753

Keyword Index 755